

\widehat{P} -matrices in orbit spaces and invariant theory

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Abstract. In many physical problems or applications one has to study functions that are invariant under the action of a symmetry group G and this is best done in the orbit space of G if one knows the equations and inequalities defining the orbit space and its strata. It is reviewed how the \widehat{P} -matrix is defined in terms of an integrity basis and how it can be used to determine the equations and inequalities defining the orbit space and its strata. It is shown that the \widehat{P} -matrix is a useful tool of constructive invariant theory, in fact, when the integrity basis is only partially known, calculating the \widehat{P} -matrix elements, one is able to determine the integrity basis completely.

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1. Introduction

In many physical applications one has to do with functions that are invariant under transformations of a compact symmetry group. These functions may be considered as functions defined on the orbit space of the group and some arguments, like the study of symmetry breaking or the study of phase transitions, are better understood if studied in the orbit space. To study invariant functions in the orbit space one has to know first the equations and inequalities that define the orbit space and its strata. A standard way to find these equations and inequalities is by using an integrity basis and the \widehat{P} -matrix. This method is reviewed in sections 2 and 4. The orbit spaces have not been widely employed in the study of invariant functions yet because the integrity basis is often unknown (the determination of an integrity basis of a general group is still an open problem of constructive invariant theory). Section 3 reviews some selected arguments of invariant theory and section 5 (the main section of this article) shows how the \widehat{P} -matrix can be used together with the Molien function to determine the integrity basis of a compact group.

2. Orbit Spaces

In this article G is a compact group acting effectively in a finite dimensional space. Then, in all generality G is a group of real orthogonal matrices acting on the real vector space \mathbf{R}^n .

The *orbit* through a point $x \in \mathbf{R}^n$ is the set: $\Omega(x) = \{g \cdot x, \forall g \in G\}$. Orbits do not intersect and define a partition of \mathbf{R}^n . The *isotropy subgroup* (or *stabilizer*) G_x of the point $x \in \mathbf{R}^n$ is the subgroup of G that leaves x unchanged: $G_x = \{g \in G \mid g \cdot x = x\}$. Isotropy subgroups of points in a same orbit are conjugated: $G_{g \cdot x} = g \cdot G_x \cdot g^{-1}$. The *orbit type* of the orbit $\Omega(x)$ is the conjugacy class $[G_x]$ of its isotropy subgroups. The orbit types define a partition of orbits (and of \mathbf{R}^n), each equivalence class $\Sigma_{[H]}$ is called a *stratum* (of \mathbf{R}^n): $\Sigma_{[H]} = \{x \in \mathbf{R}^n \mid G_x \in [H]\}$. The orbits and the strata can be partially ordered according to their orbit types. The orbit type $[H]$ is said to be *smaller* than the orbit type $[K]$: $[H] < [K]$, if $H' \subset K'$ for some $H' \in [H]$ and $K' \in [K]$. Then $[K]$ is *greater* than $[H]$. The greatest orbit type is $[G]$ and its stratum $\Sigma_{[G]}$ contains all fixed points of the G -action. $\Sigma_{[G]}$ coincides with the origin of \mathbf{R}^n if the G -action is effective. Due to the compactness of G , the number of different orbit types is finite and there is a unique smallest orbit type $[G_p]$, called the *principal* orbit type. The stratum $\Sigma_{[G_p]}$ is called the *principal stratum*, all other strata are called *singular*.

The *orbit space* is the quotient space \mathbf{R}^n/G . The natural projection $\pi : \mathbf{R}^n \rightarrow \mathbf{R}^n/G$ maps orbits of \mathbf{R}^n into single points of \mathbf{R}^n/G . Projections of strata of \mathbf{R}^n define strata of \mathbf{R}^n/G . The principal stratum of \mathbf{R}^n/G is always open connected and dense in \mathbf{R}^n/G . If $[K] > [H]$, then $\pi(\Sigma_{[K]})$ lies in the boundary of $\pi(\Sigma_{[H]})$ and the boundary of the principal stratum contains all singular strata.

A G -invariant function $f : \mathbf{R}^n \rightarrow \mathbf{R}$ is such that $f(gx) = f(x)$, $\forall g \in G$, $x \in \mathbf{R}^n$. f is then constant on the orbits and it is in fact a function defined on the orbit space.

Some symbols. $\mathbf{R}[\mathbf{R}^n]$ and $\mathbf{R}[\mathbf{R}^n]^G$ indicate the rings of real polynomial functions and of real G -invariant polynomial functions defined in \mathbf{R}^n , respectively; $\mathbf{R}[\mathbf{R}^n]_d$ and $\mathbf{R}[\mathbf{R}^n]_d^G$ indicate the rings of homogeneous polynomial functions of degree d in $\mathbf{R}[\mathbf{R}^n]$ and in $\mathbf{R}[\mathbf{R}^n]^G$, respectively; $\mathbf{R}[p_1, \dots, p_q]$ indicates the ring of polynomials with real coefficients in the q indeterminates p_1, \dots, p_q .

By Hilbert's theorem, $\mathbf{R}[\mathbf{R}^n]^G$ has a finite number q of generators [1]:

$$\forall p \in \mathbf{R}[\mathbf{R}^n]^G, \exists \widehat{p} \in \mathbf{R}[p_1, \dots, p_q] \mid p(x) = \widehat{p}(p_1(x), \dots, p_q(x)), \forall x \in \mathbf{R}^n.$$

The q generators for $\mathbf{R}[\mathbf{R}^n]^G$ are called *basic invariants* or *basic polynomials* and they form an *integrity basis* for G (and for $\mathbf{R}[\mathbf{R}^n]^G$). The integrity basis p_1, \dots, p_q is said to be *minimal* (abbreviated in MIB), if no p_a , $a = 1, \dots, q$, is a polynomial in the other elements of the basis. The basic invariants p_1, \dots, p_q may be supposed homogeneous and ordered according to their degrees d_a , for example $d_a \leq d_{a+1}$. One may choose, in all generality, $p_1(x) = \sum_{i=1}^n x_i^2$. The choice of a MIB is not unique, but the numbers q and d_a , $a = 1, \dots, q$ are uniquely determined by G .

A MIB can be used to represent the orbits as points of \mathbf{R}^q . In fact, given an orbit Ω , the vector map $p(x) = (p_1(x), p_2(x), \dots, p_q(x))$ is constant on Ω , and, given two orbits $\Omega_1 \neq \Omega_2$, $\exists p_a \in \text{MIB} \mid p_a(x_1) \neq p_a(x_2)$, $\forall x_1 \in \Omega_1, x_2 \in \Omega_2$. $p(x)$ then defines a point $p = p(x) \in \mathbf{R}^q$ that can be considered the image in \mathbf{R}^q of Ω because no other orbit is represented in \mathbf{R}^q by the same point.

The vector map: $p : \mathbf{R}^n \rightarrow \mathbf{R}^q : x \rightarrow (p_1(x), p_2(x), \dots, p_q(x))$, is called the *orbit map* and maps \mathbf{R}^n onto the subset $\mathcal{S} = p(\mathbf{R}^n) \subset \mathbf{R}^q$. p induces a one to one correspondence between \mathbf{R}^n/G and \mathcal{S} so that \mathcal{S} can be concretely identified with the orbit space of the G -action. All the strata of \mathcal{S} are images of the strata of \mathbf{R}^n through the orbit map and if $[K] > [H]$, $p(\Sigma_{[K]})$ lies in the boundary of $p(\Sigma_{[H]})$. The interior of \mathcal{S} coincides with the image of the principal stratum and the image of all singular strata lie in the bordering surface of \mathcal{S} . $p(\Sigma_{[G]})$ always coincides with the origin of \mathbf{R}^q .

Generally, the q basic invariants are algebraic dependent, that is, some polynomial $f \in \mathbf{R}[p_1, \dots, p_q]$ exists such that $f(p_1(x), \dots, p_q(x)) \equiv 0, \forall x \in \mathbf{R}^n$. In this case the polynomial $f(p_1, \dots, p_q)$ is called a *syzygy (of the first kind)*. Given a syzygy f , the equation $f(p_1, \dots, p_q) = 0$ defines a surface in \mathbf{R}^q and \mathcal{S} must be contained in that surface. So, $\mathcal{S} \subset \mathcal{Z}$, where \mathcal{Z} is the intersection of all syzygy surfaces.

All real G -invariant C^∞ -functions (not only polynomial functions) can be expressed as real C^∞ -functions of the q basic invariants of a MIB [2], and hence define C^∞ functions on \mathbf{R}^q : $f(x) = \widehat{f}(p_1(x), \dots, p_q(x)) \rightarrow \widehat{f}(p) = \widehat{f}(p_1, \dots, p_q)$. The functions $\widehat{f}(p)$ are defined also in points $p \notin \mathcal{S}$ but only the restrictions $\widehat{f}(p)|_{p \in \mathcal{S}}$ have the same range as $f(x)$, $x \in \mathbf{R}^n$. All G -invariant C^∞ functions can then be studied in the orbit space \mathcal{S} but one needs to know all equations and inequalities defining \mathcal{S} and its strata.

Details and proofs of the statements here recalled may be found in [3, 4, 5, 6] and references therein.

3. Invariant Theory

Given a MIB p_1, \dots, p_q , there are in general $s \leq q$ basic polynomials that are algebraic independent: p_{h_1}, \dots, p_{h_s} . If $s < q$ necessarily there are syzygies (of the first kind). One can determine a finite minimal set of r_1 linearly independent homogeneous polynomials, $f_1^{(1)}, \dots, f_{r_1}^{(1)} \in \mathbf{R}[p_1, \dots, p_q]$, of degrees $m_{11} \leq \dots \leq m_{1r_1}$ with respect to the natural grading assigned to the p_a ($\deg(p_a) = \deg(p_a(x))$), that generate all the syzygies of the first kind as a module over $\mathbf{R}[p_1, \dots, p_q]$. One can continue to define syzygies. Linear combinations of the r_1 variables $f_1^{(1)}, \dots, f_{r_1}^{(1)}$, with coefficients in $\mathbf{R}[p_{h_1}, \dots, p_{h_s}]$, that vanish identically by substituting the $f_i^{(1)}$ with their expressions in terms of the p_a , are called *syzygies of the second kind*. Let $f_1^{(2)}, \dots, f_{r_2}^{(2)}$ be a linearly independent basis for the syzygies of second kind, made up by homogeneous polynomials (with respect to the natural grading) of degrees $m_{21} \leq \dots \leq m_{2r_2}$. Linear combinations of the r_2 variables $f_1^{(2)}, \dots, f_{r_2}^{(2)}$, with coefficients in $\mathbf{R}[p_{h_1}, \dots, p_{h_s}]$, that vanish identically by substituting the $f_i^{(2)}$ with their expressions in terms of the $f_j^{(1)}$, are called *syzygies of the third kind*, and so on. There exist a number m such that one has syzygies of the m -th kind $f_1^{(m)}, \dots, f_{r_m}^{(m)}$, but no syzygies of the $(m+1)$ -th kind. Changing the MIB, one changes the syzygies too but does not change the numbers $q, s, m, d_a, \forall a = 1, \dots, q, r_i, m_{ij}, \forall i = 1, \dots, m, j = 1, \dots, r_i$, that are characteristic of $\mathbf{R}[\mathbf{R}^n]^G$.

By a theorem of Hochster and Roberts, in $\mathbf{R}[\mathbf{R}^n]^G$ one can choose a maximal subset of s algebraically independent polynomials: p_{h_1}, \dots, p_{h_s} , of degrees d'_1, \dots, d'_s , called *primary invariants* (or *homogeneous system of parameters*), and a number t of other homogeneous polynomials: f_1, \dots, f_t , of degrees m_1, \dots, m_t , called *secondary invariants*, such that all $p \in \mathbf{R}[\mathbf{R}^n]^G$ can be written in a unique way in following form:

$$p = \sum_{k=0}^t q_k f_k, \quad (1)$$

where $q_k \in \mathbf{R}[p_{h_1}, \dots, p_{h_s}]$, and, by definition, $f_0 = 1$ [7, 8]. In other words, all $p \in \mathbf{R}[\mathbf{R}^n]^G$ can be written in a unique way in terms of $p_{h_1}, \dots, p_{h_s}, f_0, \dots, f_t$, using the f_k at most linearly. The most convenient way to choose the p_{h_i} and the f_k is to take p_{h_1}, \dots, p_{h_s} and f_1, \dots, f_{q-s} , equal to the q basic invariants in the MIB, with $p_{h_1} = p_1$,

and f_{q-s+1}, \dots, f_t , equal to some of the products $f_k f_l$, with $1 \leq k \leq l \leq q-s$, in such a way that all products $f_k f_l$ may be expressed in the form (1) (using in case the syzygies). This choice implies that the degrees d'_l of the p_{h_l} are equal to d_a , $a \in \{h_1, \dots, h_s\}$, and the degrees m_k of the f_k are equal to d_a , $a = 1, \dots, q$, $a \notin \{h_1, \dots, h_s\}$, or to their sums. Then, the degrees m_{1l} of the syzygies of the first kind $f_l^{(1)}$ are $m_{1l} = m_i + m_j$, the degrees m_{2l} of the of the syzygies of the second kind $f_l^{(2)}$ are $m_{2l} = m_i + m_j + m_k$, and so on.

The main problem of constructive invariant theory is to determine a MIB for a given group G , and after that all the syzygies. It is then of great interest to find some algorithms that suggest what the numbers q , s , d_a , m , r_i , m_{ij} , t , m_k , are.

A key role is played by the *Molien function* $M(\eta)$ that may be calculated without the knowledge of the MIB in the following way:

$$M(\eta) = \frac{1}{|G|} \sum_{g \in G} \frac{1}{\det(e - \eta g)}, \quad \text{or} \quad M(\eta) = \int_G \frac{dg}{\det(e - \eta g)},$$

respectively for finite [7] or compact continuous [9] groups, where $\eta < 1$ is an abstract variable, e is the unit matrix of G , $|G|$ is the order of G , dg is the normalized Haar measure and the integration is over the compact group variety. The integral may be reduced to a sum of integrals over unit circles in the complex plane and calculated using the residues [10, 11]. An alternative algebraic method to compute the Molien function for compact connected groups is presented in [12].

When one calculates the Molien function from the formulas written above, one ends up with $M(\eta)$ expressed by a rational function.

The expansion of $M(\eta)$ in power series has the following interpretation:

$$M_1(\eta) = \sum_{d=0}^{\infty} \dim(\mathbf{R}[\mathbf{R}^n]_d^G) \eta^d,$$

where $\dim(\mathbf{R}[\mathbf{R}^n]_d^G)$ is the dimension of $\mathbf{R}[\mathbf{R}^n]_d^G$ as a linear space. Let's call $M_1(\eta)$ the *first form* of the Molien function. $M_1(\eta)$ gives a first information about the number and degrees of the basic invariants of small degrees. One has $\dim(\mathbf{R}[\mathbf{R}^n]_d^G) = n_d^{(0)} - n_d^{(1)} + n_d^{(2)} - \dots$, where $n_d^{(0)}$ is the number of linearly independent polynomials of degree d , $n_d^{(1)}$ is the number of linearly independent syzygies of the first kind of degree d , and so on. For sufficiently small d , one may find out the decomposition of $\dim(\mathbf{R}[\mathbf{R}^n]_d^G)$ in terms of $n_d^{(0)}$, $n_d^{(1)}$, \dots , but in general one is not able to deduce the numbers $n_d^{(i)}$.

Two rational forms of the Molien function are particularly interesting. The rational function

$$M_2(\eta) = \frac{\sum_{k=0}^t \eta^{m_k}}{\prod_{l=1}^s (1 - \eta^{d'_l})},$$

here called the *second form* of the Molien function, has the denominator that is the product of s factors of the kind $(1 - \eta^{d'_l})$, one for each primary invariant p_{h_l} , and the numerator that is a reciprocal polynomial that gives the number t of the secondary invariants f_k , and their degrees m_k .

The rational function

$$M_3(\eta) = \frac{\sum_{i=0}^m (-1)^i \sum_{j=1}^{r_i} \eta^{m_{ij}}}{\prod_{a=1}^q (1 - \eta^{d_a})},$$

here called the *third form* of the Molien function, has the denominator that is the product of q factors of the kind $(1 - \eta^{d_a})$, one for each p_a in a MIB, and the numerator that is a polynomial that gives a partial information about the number r_i of the syzygies of i -th kind $f_j^{(i)}$, and their degrees m_{ij} .

When one calculates $M(\eta)$ one ends up with a rational function that is generally different from both $M_2(\eta)$ and $M_3(\eta)$. To get $M_2(\eta)$ and $M_3(\eta)$ from $M(\eta)$ one has to multiply numerator and denominator of $M(\eta)$ by convenient factors. Obviously, one has $M(\eta) = M_1(\eta) = M_2(\eta) = M_3(\eta)$.

If G is finite then $s = n$. If G is a compact Lie group then $s = n - \dim G + \dim G_p$.

The expressions for $M_2(\eta)$ and $M_3(\eta)$ coincide only if $q = s$ (and this implies $t = m = 0$). Many groups for which $q = s$ are classified in [13, 14, 15, 16].

In the general case $s < q$, $M_2(\eta)$ and $M_3(\eta)$ are unknown as long as one does not know the MIB completely. A possible expression for $M_2(\eta)$ can easily be found by requiring only positive coefficients in the numerator. At this point other possible expressions for $M_2(\eta)$ are obtained by multiplying the numerator and the denominator of $M_2(\eta)$ by factors like $(1 + \eta^{d'_i})$, where d'_i appears in the exponents of the denominator, increasing in this way the number of secondary invariants required by the numerator. Generally, when one starts to calculate the MIB, one knows the number s of algebraically independent polynomials, so one is able to write down the correct form for $M_2(\eta)$. For a given expression of $M_2(\eta)$, one has to guess the correct expression of $M_3(\eta)$. One notes that:

- (i) One obtains $M_3(\eta)$ by multiplying numerator and denominator of $M_2(\eta)$ by a certain (unknown) number $(q - s)$ of factors like $(1 - \eta^{d_a})$, one for each basic non-primary invariant f_k , $k = 1, \dots, q - s$ (and this implies the equality $m = q - s$).
- (ii) The coefficients in the numerator of $M_3(\eta)$ corresponding to the syzygies of the first kind are negative.
- (iii) An invariant f_k , whose degree m_k appears in the numerator of $M_2(\eta)$, must coincide or with a basic non-primary invariant, or with a product of them. This implies that: (i) for each f_k , whose degree m_k cannot be written as a sum of degrees of basic polynomials, there is a factor $(1 - \eta^{m_k})$ in the denominator of $M_3(\eta)$; (ii) the degrees of the syzygies of the first kind are $m_{1j} \geq 2m_1$.

If one does not know the numbers q and d_a , there are many “possibly right” expressions for $M_3(\eta)$ that satisfy all the points written above, but only one is the correct one, corresponding to the right numbers q and d_a . Moreover, given the right expression for $M_3(\eta)$, the numbers m , r_i , m_{ij} , are not immediately readable from the numerator because of simplifications between similar terms. In any case, if there is only one kind of syzygies of degree d (for example if d is small), the coefficient of η^d in the numerator allows to know the number of independent syzygies of degree d .

Summarizing, the Molien function is a first powerful device to study $\mathbf{R}[\mathbf{R}^n]^G$ because it gives some information about the degrees d_a and allows, in any case, to determine correctly the number and degrees of the basic invariants of small degrees.

When one knows the degrees of some invariants, one may find them explicitly using known properties of the group action or by means of the classical procedure of averaging in the group. Given an arbitrary function $f(x)$, its average in the group is the invariant function $F(x)$, where:

$$F(x) = \frac{1}{|G|} \sum_{g \in G} f(gx), \quad \text{or} \quad F(x) = \int_G f(gx) \, dg,$$

respectively for finite [17] or continuous compact [18] groups. Obviously, for the linearity of G , if $f(x) \in \mathbf{R}[\mathbf{R}^n]_d$, then $F(x) \in \mathbf{R}[\mathbf{R}^n]_d^G$, so to get an invariant of degree d one may take the average in the group of a monomial of degree d . If d and n are small, one has only a limited number of possible choices of monomials of degree d , but, if d or n are great, this averaging procedure becomes difficult to carry out, because of the many possible monomials of degree d one may choose to average and because most of the invariants that one finds out in this way are not independent from those that one already knows.

For a detailed presentation of invariant theory and for the proofs that are here omitted, the interested reader may read [1, 7, 10, 11, 19, 20, 21] and the references therein.

4. \hat{P} -matrices and Orbit Spaces

Given a stratum $\Sigma \subset \mathbf{R}^n$, in a point $x \in \Sigma$, the number of linear independent gradients of the basic invariants is equal to the dimension of the stratum $p(\Sigma) \subset \mathcal{S}$ [22]. One may calculate the $q \times q$ Grammian matrix $P(x)$ with elements $P_{ab}(x)$ that are scalar products of the gradients of the basic invariants [23]:

$$P_{ab}(x) = \nabla p_a(x) \cdot \nabla p_b(x) = \sum_{i=1}^n \frac{\partial p_a(x)}{\partial x_i} \frac{\partial p_b(x)}{\partial x_i},$$

so, if $x \in \Sigma$, $\text{rank}(P(x)) = \dim(p(\Sigma))$.

From the covariance of the gradients of G -invariant functions ($\nabla f(g \cdot x) = g \cdot \nabla f(x)$) and the orthogonality of G , the matrix elements $P_{ab}(x)$ are G -invariant homogeneous polynomial functions of degree $d_a + d_b - 2$, so they may be expressed as polynomials of the basic invariants:

$$P_{ab}(x) = \hat{P}_{ab}(p_1(x), \dots, p_q(x)) = \hat{P}_{ab}(p) \quad \forall x \in \mathbf{R}^n \text{ and } p = p(x).$$

One can define then a matrix $\hat{P}(p)$ in \mathbf{R}^q , called a \hat{P} -matrix, having $\hat{P}_{ab}(p)$ for elements. At the point $p = p(x) \in \mathcal{S}$, image in \mathbf{R}^q of the point $x \in \mathbf{R}^n$ through the orbit map, the matrix $\hat{P}(p)$ is the same as the matrix $P(x)$, $\hat{P}(p)$ is however defined in all \mathbf{R}^q , also outside \mathcal{S} , but only in \mathcal{S} it reproduces $P(x)$, $\forall x \in \mathbf{R}^n$.

$\hat{P}(p)$ is a real, symmetric $q \times q$ matrix and its matrix elements $\hat{P}_{ab}(p)$ are homogeneous polynomial functions of degree $d_a + d_b - 2$ with respect to the natural grading, $\text{rank}(\hat{P}(p))$ is equal to the dimension of the stratum containing p , and \mathcal{S} is the *only* region of \mathcal{Z} where $\hat{P}(p)$ is positive semidefinite [6, 24].

If $s \leq q$ basic invariants are algebraic independent, one has $\text{rank}(\hat{P}(p)) = s$, $\forall p$ in the principal stratum, and \mathcal{S} has dimension s .

The matrix $\hat{P}(p)$ completely determines \mathcal{S} and its stratification. Defining \mathcal{S}_k the union of all k -dimensional strata of \mathcal{S} , ($k = 1, \dots, s$), one has:

$$\mathcal{S} = \{p \in \mathcal{Z} \mid \hat{P}(p) \geq 0\}, \quad \mathcal{S}_k = \{p \in \mathcal{Z} \mid \hat{P}(p) \geq 0, \text{rank}(\hat{P}(p)) = k\}$$

To find out the defining equations and inequalities of k -dimensional strata, one may impose that all the principal minors of $\hat{P}(p)$ of order greater than k are zero and that at least one of those of order k , and all those of order smaller than k are positive.

The \hat{P} -matrix contains all information necessary to determine the geometric structure of the orbit space and its strata, so, if one wishes to classify geometrically the orbit spaces, it is sufficient to classify the \hat{P} -matrices. This, in turn, gives a non-standard group classification. One discovers so that different groups, no matter if finite or continuous, share the same orbit space structure, despite the fact that the strata correspond to different orbit types (some examples are in Table X of [25]). They exist different MIB's (of different linear groups), with the same number of invariants and the same degrees, that determine: (i) the same \hat{P} -matrix (some examples are in Table X of [25]); (ii) different \hat{P} -matrices (an example is given by Entries 6 and 25 of Table V of [25]).

Some examples using the \hat{P} -matrices to study orbit space stratifications, minima of invariant polynomials and phase transitions may be found in [26, 25, 27].

5. \hat{P} -matrices and Invariant Theory

The \hat{P} -matrix method to determine a MIB is summarized in the following items (i)-(iv) and applied in three examples.

Let p_1, \dots, p_q be a set of q independent G -invariant homogeneous polynomials.

- (i) With p_1, \dots, p_q one tries to construct the \hat{P} -matrix. By Euler's theorem on homogeneous functions and the standard choice for p_1 , one has $\hat{P}_{1a}(p) = \hat{P}_{a1}(p) = 2d_a p_a$, $\forall a = 1, \dots, q$. Taking into account the symmetry of $\hat{P}(p)$, one has then to calculate only the matrix elements $\hat{P}_{ab}(p)$, with $2 \leq a \leq b \leq q$.
- (ii) If it is not possible to express $P_{ab}(x)$ as a polynomial in $p_1(x), \dots, p_q(x)$, then $P_{ab}(x)$ is an invariant of degree $d_a + d_b - 2$ that is independent from the known ones. One has then to add a new basic invariant to the set p_1, \dots, p_q . One may choose, for example, an irreducible invariant factor of $P_{ab}(x)$ independent from p_1, \dots, p_q .
- (iii) When one succeeds to express all the matrix elements $P_{ab}(x)$ in term of the basic invariants, one has found a "closed" \hat{P} -matrix $\hat{P}(p)$ and a set p_1, \dots, p_q that is a MIB (or part of it) for a group \hat{G} that either coincides with G or contains G as a subgroup (see Example 3).
- (iv) To check if p_1, \dots, p_q do form a complete MIB for G one has to look to the Molien function of G . If $M_2(\eta)$ and $M_3(\eta)$ agree with the MIB p_1, \dots, p_q , then this is the MIB for G one was searching in. If instead $M_3(\eta)$ requires a different set of degrees for the basic polynomials, then one has to find out (by averaging in the group or in some other way) at least one of the missing basic polynomials of the lowest degree. If p_0 is this new invariant, first of all one has to check if the higher degree invariants in the set p_1, \dots, p_q are all independent from p_0 , otherwise one has to discard the non independent ones. Then, return to item (i) above with p_0 in the set of the q invariant polynomials.

Some technical suggestions. With the \hat{P} -matrix method, with only invariants of degree 2 one is not able to determine higher degrees invariants and with only even degree invariants one is not able to determine odd degree invariants. So it is convenient to start to build the \hat{P} -matrix having determined in some way at least all invariants of degree 2, all invariants of the smallest odd degree and all the invariants of the smallest even degree greater than 2. One then starts to determine the \hat{P} -matrix as indicated

in items (i)-(iv) above, proceeding step after step to calculate the matrix elements of increasing degrees. During this calculation, every time one adds a basic invariant to the set of basic invariants p_1, \dots, p_q , according to item (ii) above, it is convenient to look if this MIB is consistent with the guessed expression of $M_2(\eta)$ and $M_3(\eta)$. In case, one has to modify the expressions of $M_2(\eta)$ and/or $M_3(\eta)$ to include the new basic invariant. One has so a partial check of the correctness either of $M_2(\eta)$ and $M_3(\eta)$, either of the MIB. Every time one starts to determine the matrix elements $\hat{P}_{ab}(p)$ of a given degree d , it is convenient to control if one knows explicitly all the basic invariants of degree lower than d that are predicted by $M_3(\eta)$. If one misses one of these invariants it is strongly recommended to find out this basic invariant first, otherwise, one does longer and harder calculations.

If a subset p_{l_1}, \dots, p_{l_k} of the MIB for G is a complete MIB for a group $\hat{G} \subseteq O(n, \mathbf{R})$, containing G as a subgroup, then the principal minor of the \hat{P} -matrix of G formed by the rows and columns l_1, \dots, l_k is expressed only in terms of p_{l_1}, \dots, p_{l_k} .

Example 1. Let $G = O_h$, the symmetry group of the cube. The Molien function of G has the following expression:

$$M_2(\eta) = M_3(\eta) = \frac{1}{(1 - \eta^2)(1 - \eta^4)(1 - \eta^6)}$$

and predicts a MIB with 3 algebraic independent polynomials of degree 2, 4 and 6 that have been calculated by many authors (see for ex. Table 4 of [5]). As an elementary example of the \hat{P} -matrix method to determine a MIB, let us start with the basic invariants $p_1 = x^2 + y^2 + z^2$ and $p_2 = x^4 + y^4 + z^4$. The only non trivial element of the \hat{P} -matrix formed with p_1 and p_2 is \hat{P}_{22} . One finds easily $\nabla p_2 = (4x^3, 4y^3, 4z^3)$ and $P_{22} = \nabla p_2 \cdot \nabla p_2 = 16(x^6 + y^6 + z^6)$. As \hat{P}_{22} cannot be written in the form $c_1 p_1^3 + c_2 p_1 p_2$, the basis p_1 and p_2 is not complete and one may take $p_3 = x^6 + y^6 + z^6$ for a third element of the MIB. All elements of the \hat{P} -matrix constructed with p_1 , p_2 and p_3 can be written only in terms of p_1 , p_2 and p_3 , so the MIB is complete, it agrees with the Molien function and in fact is a possible MIB for G . This trivial Example shows that by constructing the \hat{P} -matrix with only part of the MIB known, one succeeds to find out all the missing basic invariants.

Example 2. Let G be the group of order 192 generated by the matrices

$$g_1 = \frac{\sqrt{2}}{2} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{pmatrix}, \quad g_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}.$$

This group is the realification of the complex unitary group considered in [19], and one is referred to [19] for details about its structure.

The Molien function of G has the following first and second form:

$$\begin{aligned} M_1(\eta) &= 1 + \eta^2 + \eta^4 + \eta^6 + 4\eta^8 + 4\eta^{10} + 7\eta^{12} + 7\eta^{14} + 12\eta^{16} + \\ &\quad + 17\eta^{18} + 22\eta^{20} + 22\eta^{22} + 36\eta^{24} + 43\eta^{26} + \dots, \\ M_2(\eta) &= \frac{1 + 2\eta^8 + 2\eta^{12} + 2\eta^{16} + 5\eta^{18} + 5\eta^{24} + 2\eta^{26} + 2\eta^{30} + 2\eta^{34} + \eta^{42}}{(1 - \eta^2)(1 - \eta^8)(1 - \eta^{12})(1 - \eta^{24})}. \end{aligned}$$

From $M_1(\eta)$ one gets the following kind of information. The term $4\eta^8$ suggests that there are 4 lin. indep. invariants of degree 8: p_1^4, p_2, p_3, p_4 . The term $7\eta^{12}$ suggests that there are 7 lin. indep. invariants of degree 12: $p_1^6, p_1^2p_2, p_1^2p_3, p_1^2p_4, p_5, p_6, p_7$. The term $12\eta^{16}$ suggests that there are 12 lin. indep. invariants of degree 16: 13 lin. indep. invariants are the terms in the expansion of the polynomial $(p_2 + p_3 + p_4 + p_1^4)^2 + (p_5 + p_6 + p_7)p_1^2$ and it must exist one syzygy of the first kind of degree 16, $f_1^{(1)}$, so that $12 = 13 - 1$. The term $17\eta^{18}$ suggests that there are 17 lin. indep. invariants of degree 18: 12 independent invariants are found by multiplying by p_1 the 12 independent invariants of degree 16, and there must exist 5 new basic invariants of degree 18: $p_8, p_9, p_{10}, p_{11}, p_{12}$, so that $17 = 12 + 5$. One may continue this analysis and find out that there are 4 syzygies of the first kind of degree 20: $f_2^{(1)}, \dots, f_5^{(1)}$ and no basic invariants and no syzygies of degree 22. The analysis becomes very uncertain for degree 24 because one might have either basic invariants, either syzygies of the first and of the second kind, and one only knows that their numbers $n_{24}^{(0)}, n_{24}^{(1)}$ and $n_{24}^{(2)}$ must satisfy the condition $n_{24}^{(0)} - n_{24}^{(1)} + n_{24}^{(2)} = 36$.

The information obtained so far from $M_1(\eta)$ and $M_2(\eta)$ suggest to obtain the third form of the Molien function by multiplying numerator and denominator of $M_2(\eta)$ by $(1 - \eta^8)^2(1 - \eta^{12})^2(1 - \eta^{18})^5$. Note that the exponents 2, 2, 5 are the coefficients of $\eta^8, \eta^{12}, \eta^{18}$ in the numerator of the second form of the Molien function. Doing this, one finds a third form of the Molien function that shows at the numerator the existence of the syzygies $f_1^{(1)}, \dots, f_5^{(1)}$ but suggests, wrongly, that there is only one basic invariant of degree 24. At this point it is convenient to stop the (uncertain) analysis of the Molien function and start to build the \hat{P} -matrix.

The Molien function suggests so far a MIB with 1 invariant of degree 2: p_1 , 3 invariants of degree 8: p_2, p_3, p_4 , 3 invariants of degree 12: p_5, p_6, p_7 , 5 invariants of degree 18: $p_8, p_9, p_{10}, p_{11}, p_{12}$, and one invariant of degree 24: p_{13} . In this example the explicit calculation of all the invariants by the method of averaging in the group is not trivial, because of the high degree of the invariants, so, it is convenient to use the \hat{P} -matrix method.

First of all, one defines: $p_1(x) = x_1^2 + x_2^2 + x_3^2 + x_4^2$ and finds out the three invariants of degree 8, for example by averaging in the group the monomials $x_1^2x_2^2x_3^2x_4^2, x_1^4x_3^4$ and $x_1^5x_3^3$. One then starts to build up the \hat{P} -matrix. One calculates first the matrix elements of degree 14: $P_{2,2}(x), \dots, P_{4,4}(x)$ and one finds out the 3 basic invariants of degree 12. One then calculates the matrix elements of degree 18: $P_{2,5}(x), \dots, P_{4,7}(x)$, and one finds out the 5 basic invariants of degree 18. One then calculates the matrix elements of degree 22: $P_{5,5}(x), \dots, P_{7,7}(x)$, with no need of new basic invariants. One then calculates the matrix elements of degree 24: $P_{2,8}(x), \dots, P_{4,12}(x)$, and one finds out two basic invariants of degree 24: $p_{13}(x)$ and $p_{14}(x)$, not only one, as expected. Then the third form of the Molien function has to be corrected by multiplying its numerator and denominator by $(1 - \eta^{24})$ and obtaining:

$$M_3(\eta) = \frac{1 - \eta^{16} - 4\eta^{20} - \eta^{24} - 8\eta^{26} + 4\eta^{28} - 8\eta^{30} + 8\eta^{34} - 19\eta^{36} + \dots}{(1 - \eta^2)(1 - \eta^8)^3(1 - \eta^{12})^3(1 - \eta^{18})^5(1 - \eta^{24})^2}.$$

Calculating all the remaining elements of the \hat{P} -matrix one does not need any new basic invariant. As p_1, \dots, p_{14} agrees with the third form of the Molien function, they form a complete MIB for G . It is important to note that the invariant p_{14} was not

predicted from the Molien function, but it is required to express some of the elements of the matrix $P(x)$ in terms of the MIB.

This example shows that the Molien function is not sufficient to specify the number and degrees of all the basic invariants in a MIB, but its combined use with the construction procedure of the \hat{P} -matrix allows one to do that. Moreover, the \hat{P} -matrix method is constructive, in the sense that it allows to determine concretely the MIB.

In this case no proper subset of the MIB p_1, \dots, p_{14} , is a complete MIB for a group \hat{G} containing G as a subgroup, because no principal minor of the \hat{P} -matrix can be written only in terms of the corresponding subset of basic invariants.

Having found the MIB, all the syzygies of any kind can be determined.

Example 3. Let G be the cyclic group of order 3, generated by the matrix

$$g = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}.$$

The three forms of the Molien function are easily found. The second form is

$$M_2(\eta) = \frac{1 + \eta^3}{(1 - \eta^2)(1 - \eta^3)}$$

and suggests a MIB of 3 elements of degree 2, 3, 3. Using the standard form of p_1 and averaging the monomials x_1^3 and x_2^3 , one finds out the following MIB:

$$p_1 = x_1^2 + x_2^2, \quad p_2 = x_1^3 - 3x_1x_2^2, \quad p_3 = x_2^3 - 3x_2x_1^2.$$

If one uses the \hat{P} -matrix method in this trivial example starting with the basic invariants p_1 and p_2 , one does not need any other invariant to write down the \hat{P} -matrix and would not find p_3 . The group that leaves p_1 and p_2 invariant however is G , that has 3 invariants, according to its Molien function. To use the \hat{P} -matrix method it is then necessary to start with all invariants of the smaller degree greater than 2.

Let now H be the cyclic group of order 3, generated by the 4×4 matrix

$$h = \begin{pmatrix} g & e \\ e & g \end{pmatrix},$$

where e is the unit matrix of order 2 and g is the matrix written above. The three forms of the Molien function are easily found. The second form is

$$M_2(\eta) = \frac{1 + 2\eta^2 + 6\eta^3 + 2\eta^4 + \eta^6}{(1 - \eta^2)^2(1 - \eta^3)^2},$$

and suggests a MIB of 12 elements: p_1, \dots, p_4 of degree 2, and p_5, \dots, p_{12} of degree 3. All the basic invariants can be easily found by averaging in the group. For example, one may use the standard form of p_1 and the averages of the monomials $x_1^2, x_1x_3, x_1x_4, x_1^3, x_2^3, x_3^3, x_4^3, x_1x_2x_3, x_1x_2x_4, x_1x_3x_4, x_2x_3x_4$ for the invariants p_2, \dots, p_{12} . One verifies easily that none of them can be expressed as a polynomial in the other ones, so they form a MIB for H .

In this case if one uses the \hat{P} -matrix method starting with p_1, \dots, p_4 and one arbitrary invariant of degree 3 one would also find out all the basic polynomials of

a MIB (generally with more complicated expressions than those obtained from the averages).

If one uses the \widehat{P} -matrix method starting for example with the basic invariants $p_1 = x_1^2 + x_2^2 + x_3^2 + x_4^2$, $p_2 = x_1^2 + x_2^2$ and $p_5 = x_1^3 - 3x_1x_2^2$, one does not need any other invariant to write down the \widehat{P} -matrix. One knows from the Molien function that the polynomials p_1, p_2, p_5 do not form a MIB for H and one understands that one has to use more invariants at the beginning to find out the MIB with the \widehat{P} -matrix method. The invariance group of p_1, p_2, p_5 is the group \widehat{H} , containing H as a subgroup, generated by an arbitrary rotation in the plane x_3, x_4 and by the matrix g acting in the plane x_1, x_2 . We know from above, or from the Molien function of \widehat{H} :

$$M_2(\eta) = \frac{1 + \eta^3}{(1 - \eta^2)^2(1 - \eta^3)},$$

that a MIB for \widehat{H} has 2 invariants of degree 2 and 2 of degree 3, so p_1, p_2, p_5 is not a complete MIB even for \widehat{H} .

This example suggests that it is convenient to start using the \widehat{P} -matrix method after having determined all invariants of degree 2 and all invariants of the smaller degree greater than 2 predicted by the Molien function. Moreover, it shows that the Molien function plays a fundamental role to decide if a given set of invariants do form a complete MIB for some group or not.

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